Asphalt Research Consortium

Chemomechanical Approaches to Predict Asphalt Pavement Behavior and Performance

Troy Pauli, Western Research Institute
Linbing Wang and Wenjuan Sun,
Virginia Polytechnic Institute

"ARC Deliverables/Products Presentation and Workshop"

TRB 2015, Thursday, January 15, 2015, 9:00am - 5:00pm,
Marriott Marquis, Washington DC.

Acknowledgements

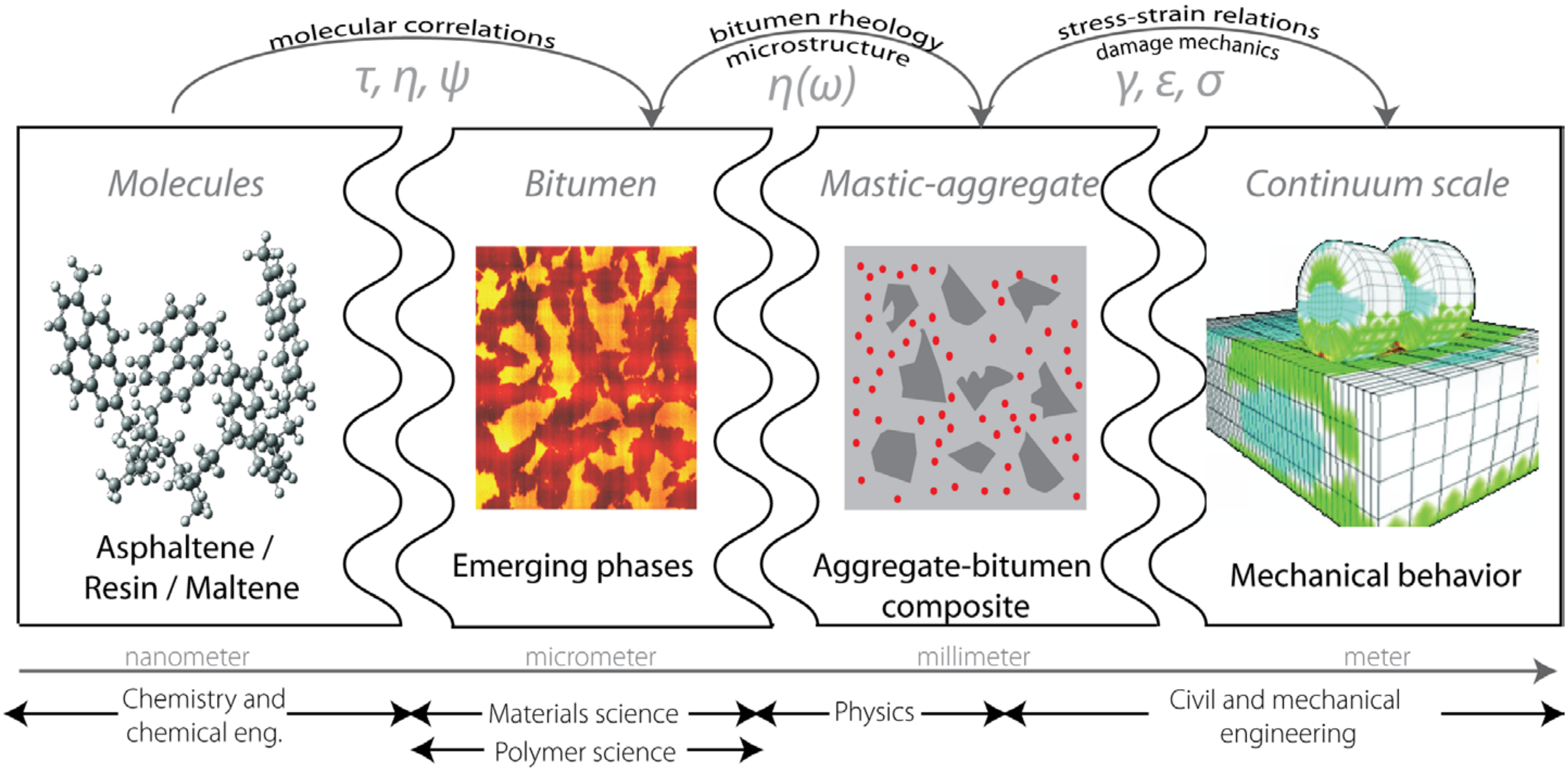
This research has been supported by

Federal Highway Administration
U. S. Department of Transportation
Under Cooperative Agreement
No. DTFH61-07-H-00009

Delft University of Technology
Faculty of Civil Engineering and Geosciences
Section of Road and Railway Engineering

& The Delft Healing Consortium

Asphalt Microstructure Model Team



Asphalt Microstructure Model Team

- Asphalt composition (chemistry) drives binder rheological behavior, which in turn drives mechanical (performance) behavior.
- Crude source dictates asphalt composition (chemistry) but may be modified to produce desired rheological and mechanical (performance) behavior.
- Crude source variation hinders prediction of pavement behavior.
- Fundamental theories of material properties coupled with multi-scale modeling efforts implemented now insures that the technology needed to effectively modify and model asphalt pavement behavior will be available in the future.

Asphalt Microstructure Model Team

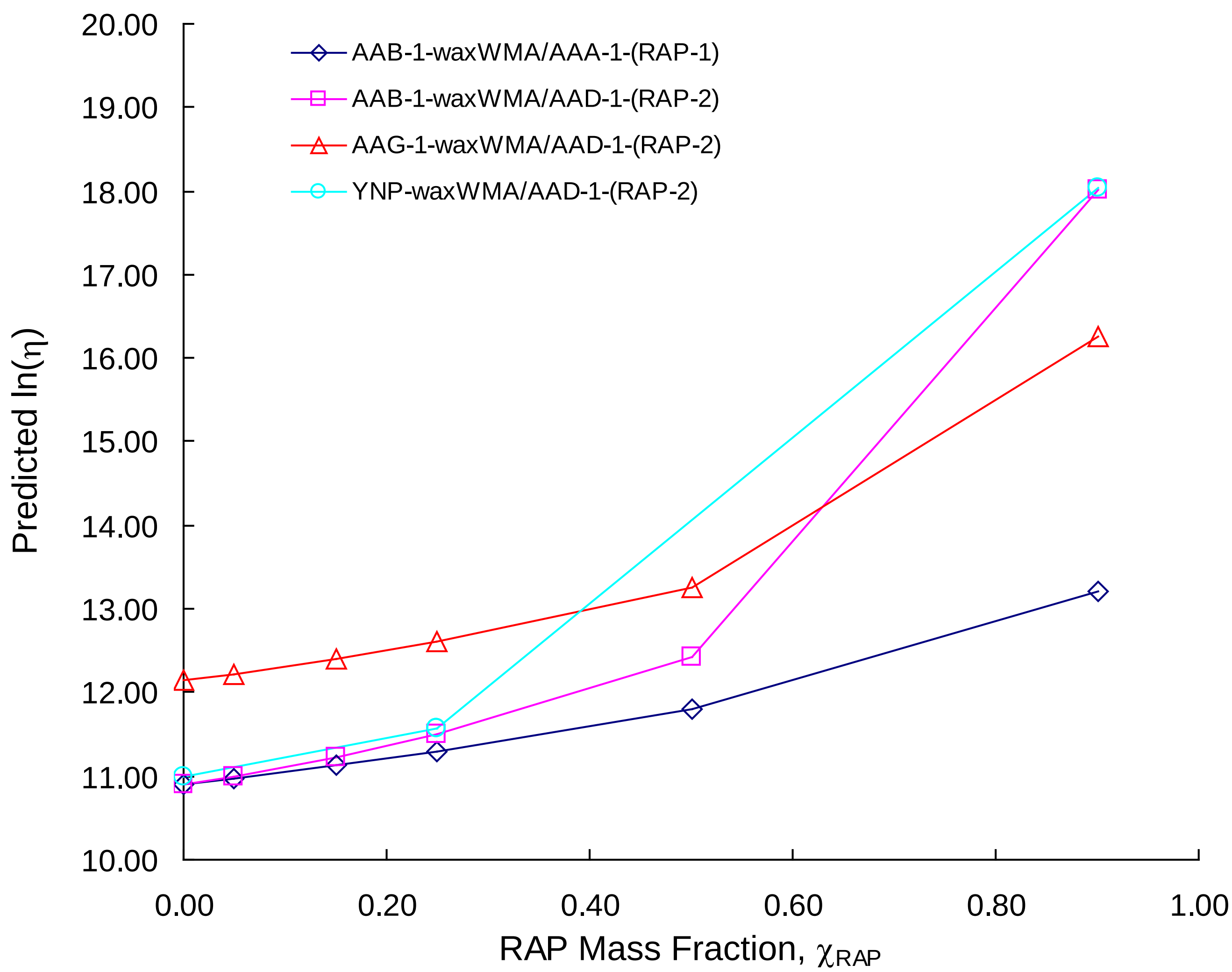
- Multiscale modeling endeavors provide a link between fundamental material properties and mechanical (performance) properties.
- A chemomechanical theory of asphalt binder behavior has developed which integrates asphalt composition (chemistry) to physicochemistry and binder rheology, which relates to pavement mechanical behavior.
- A deliverable of this research is source code of phase-behavior of asphalt binder (i.e., asphalt composition (chemistry)) which is compatible with finite element methods to predict mechanical response.
- A chemomechanical modeling platform will provide chemical, physical and rheological input parameters for finite element models based on fundamental material properties and theories.

Asphalt Research Consortium

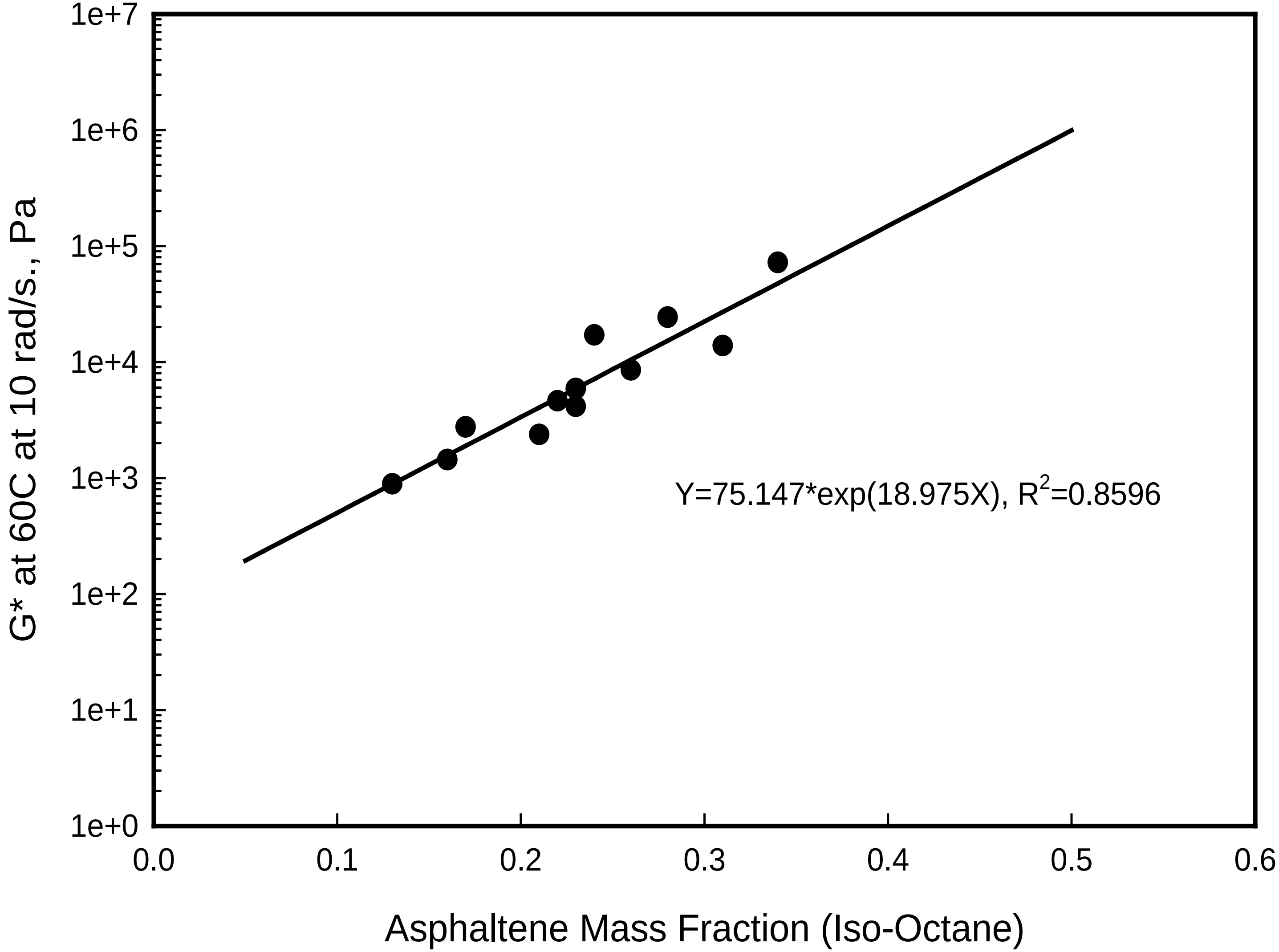
Physicochemical Model of RAP Blending

Prediction of RAP Asphalt Flow

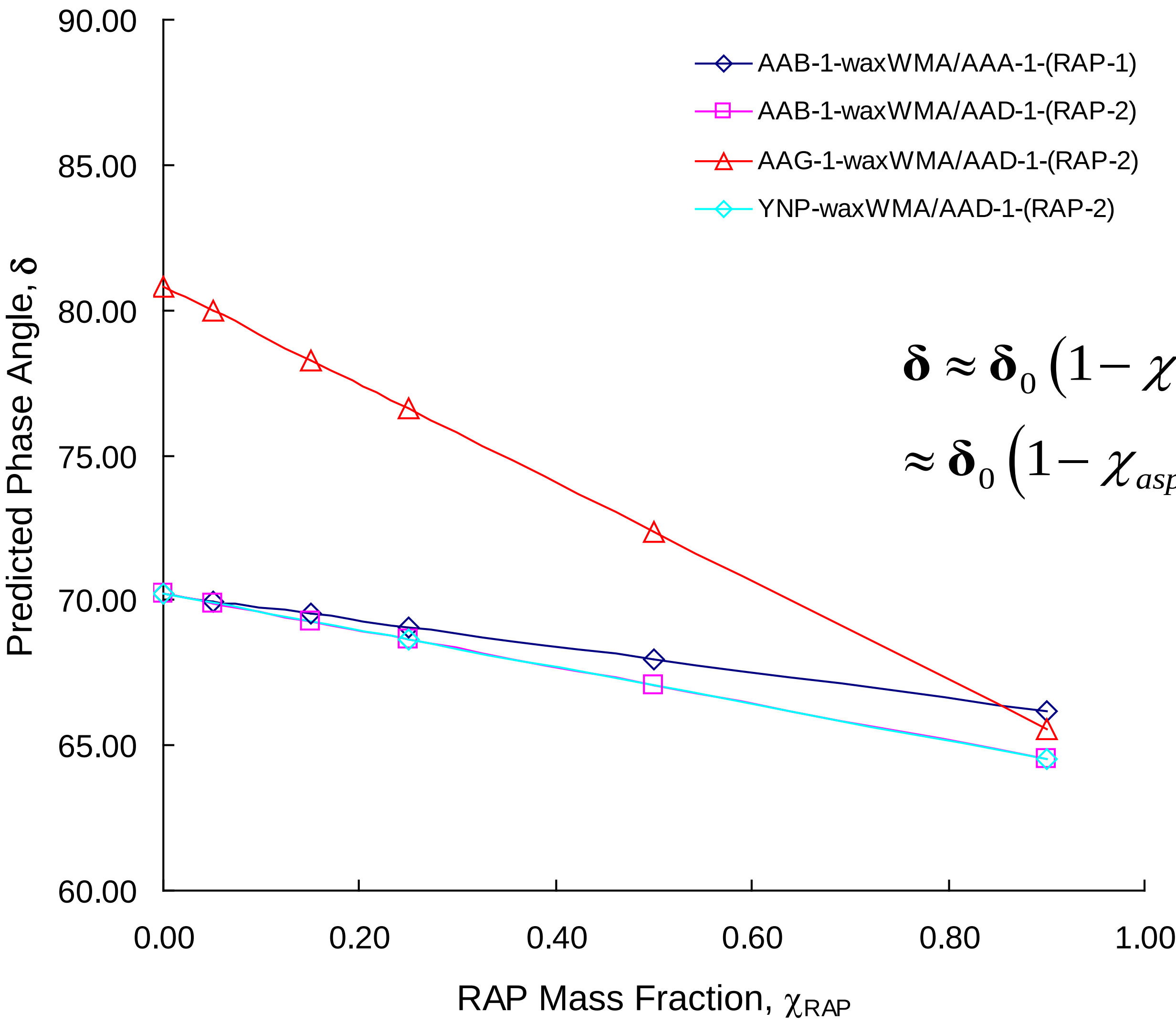
$$\eta_{blend} = \left(x_{RAP}\left(\eta_0\right)_{RAP} + x_{neat}\left(\eta_0\right)_{neat}\right)\left(1 - K_{blend}\left(x_{RAP}\left(x_a\right)_{RAP} + x_{neat}\left(x_a\right)_{neat}\right)\right)^{-2.5}$$



RAP-Asphalt Flow Properties



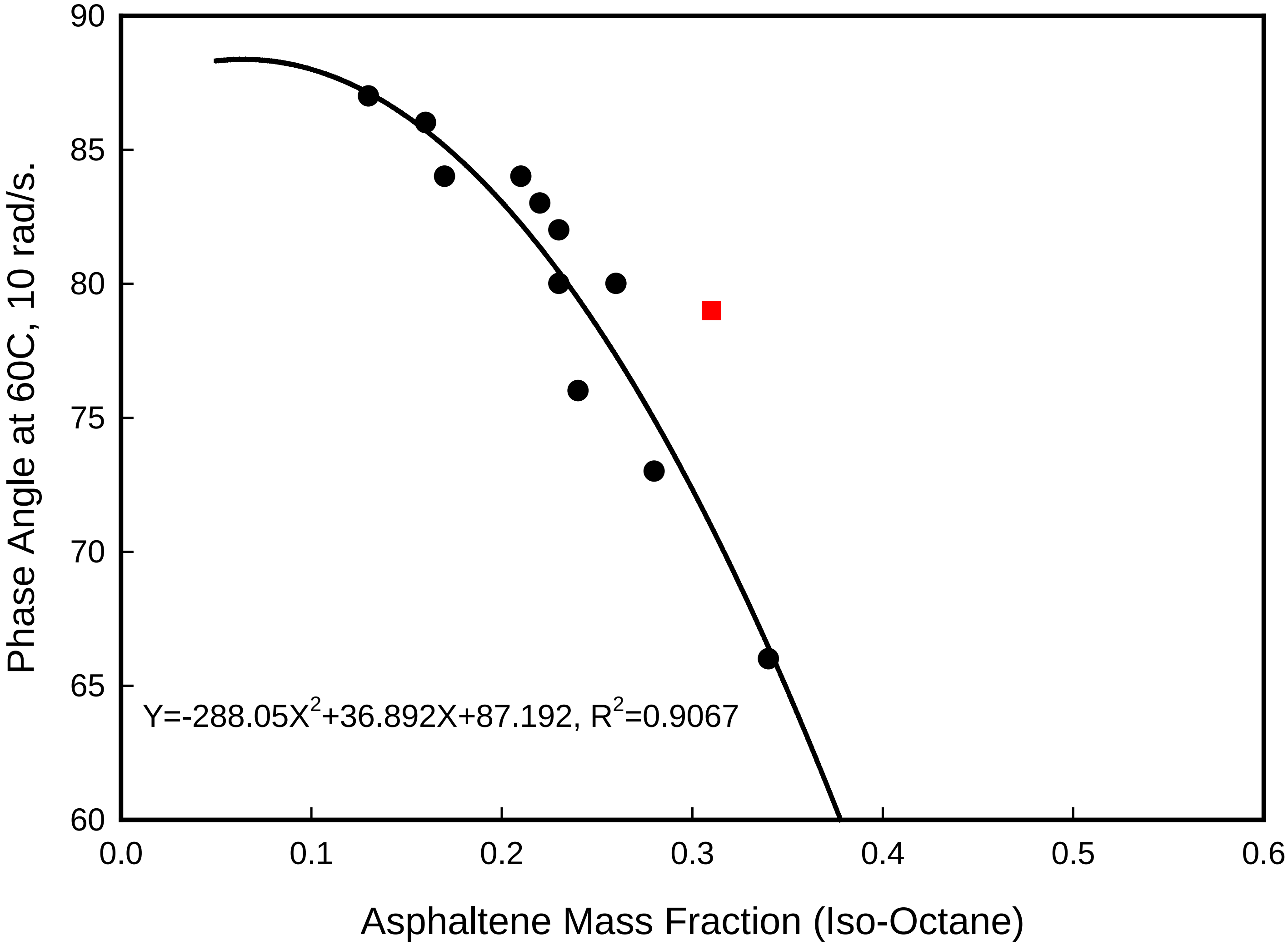
Prediction of RAP Asphalt Flow



$$\boldsymbol{\delta} \approx \boldsymbol{\delta}_0 \left(1 - \chi_{SECI}\right)$$

$$\approx \boldsymbol{\delta}_0 \left(1 - \chi_{asphaltene}\right)$$

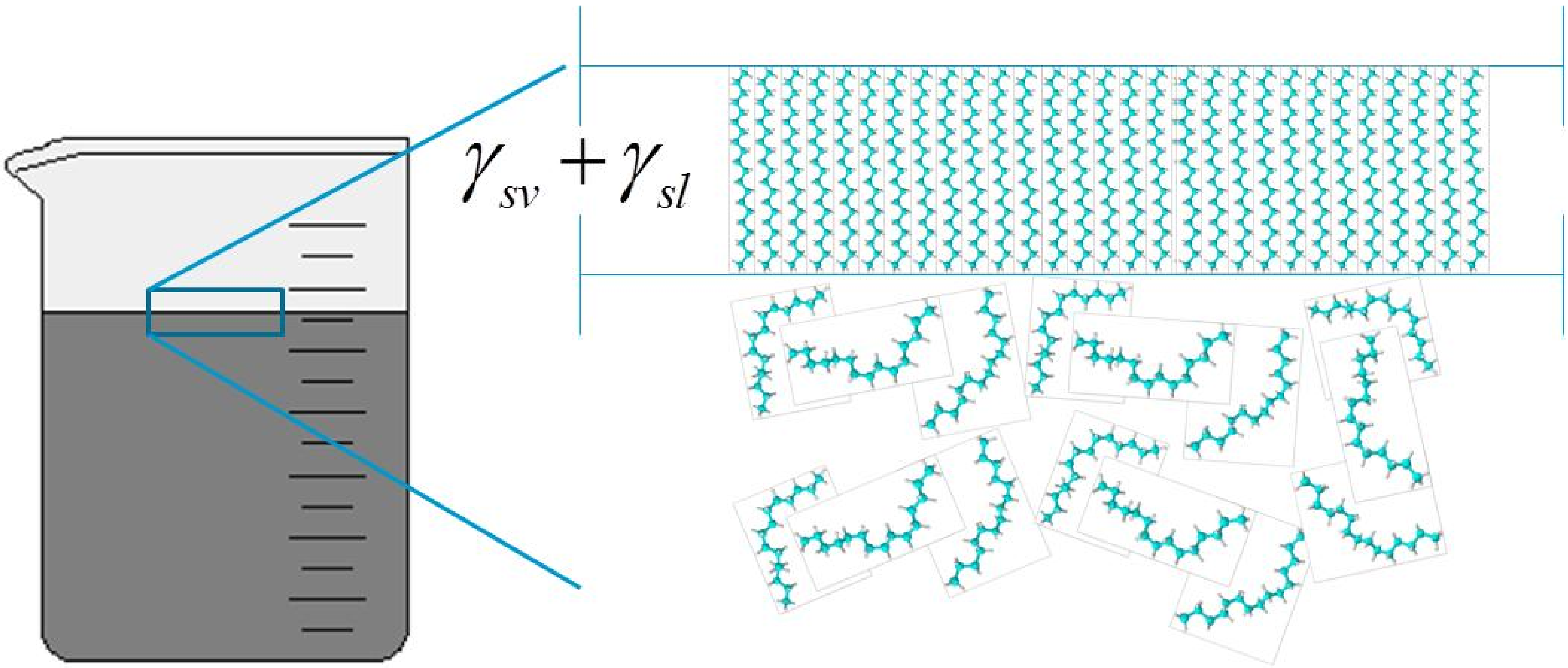
RAP-Asphalt Flow Properties



Physicochemical Model of Wax Surface Structuring

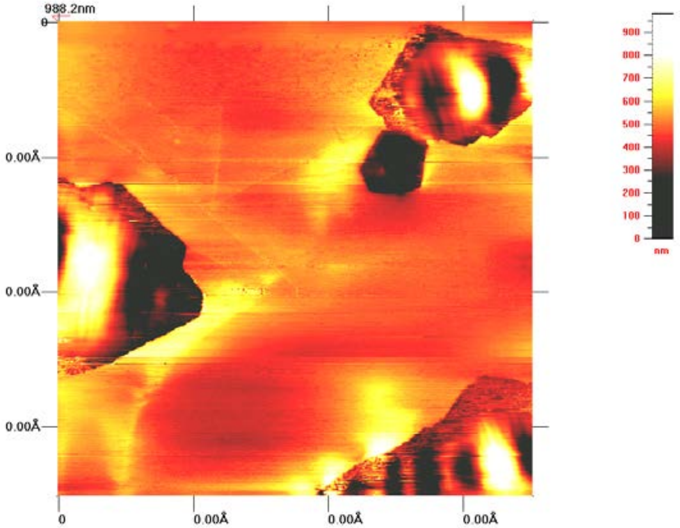
Wax Surface-Freezing in Complex Media

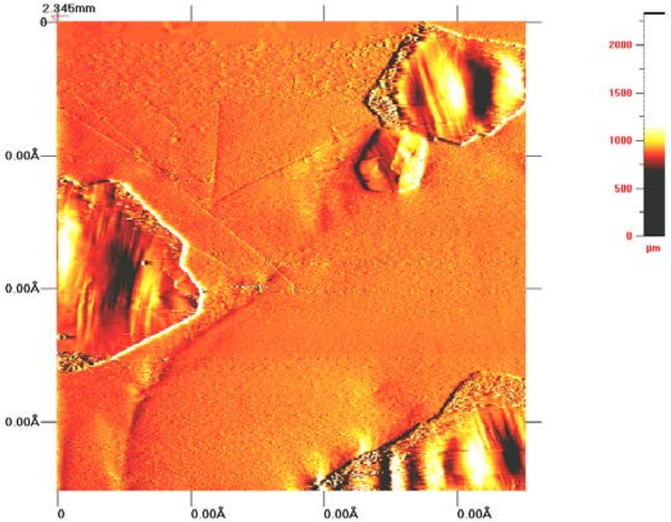
Paraffin surface freezing "detected" by
X-ray reflectivity and grazing incidence diffraction



X.Z. Wu, B.M. Ocko, E.B. Sirota, S.K. Sinha, M. Deutsch, B.H. Cao, M.W. Kim, Surface Tension Measurements of Surface Freezing in Liquid Normal Alkanes, *Science*, 261 (1993a) 1018-1020.

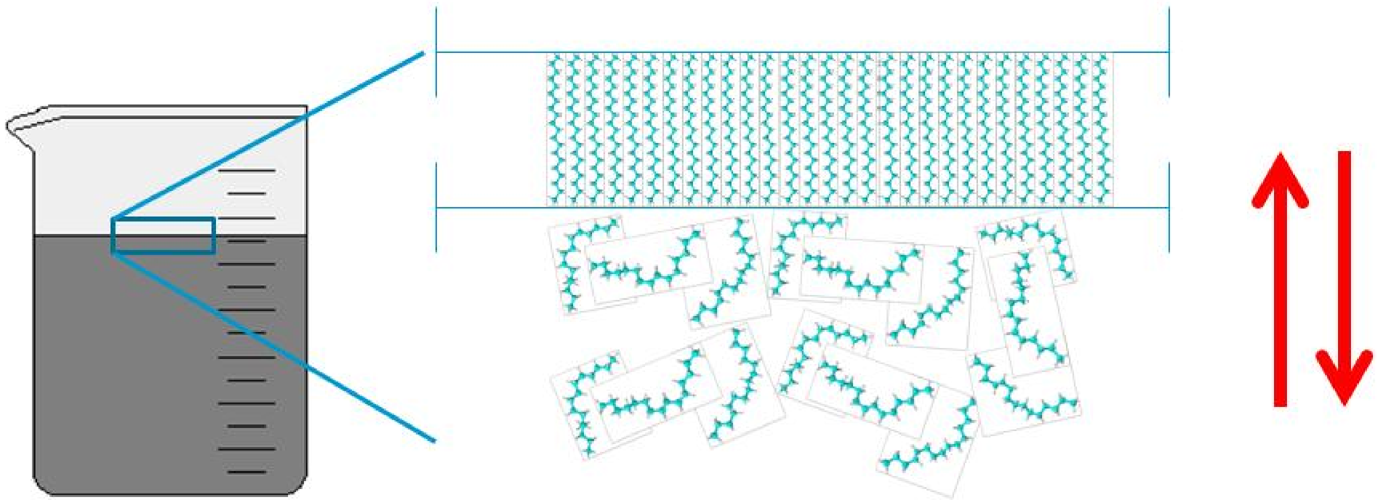
Artificial Bees: Paraffin in paraffin oil





Wax Surface-Freezing in Complex Media

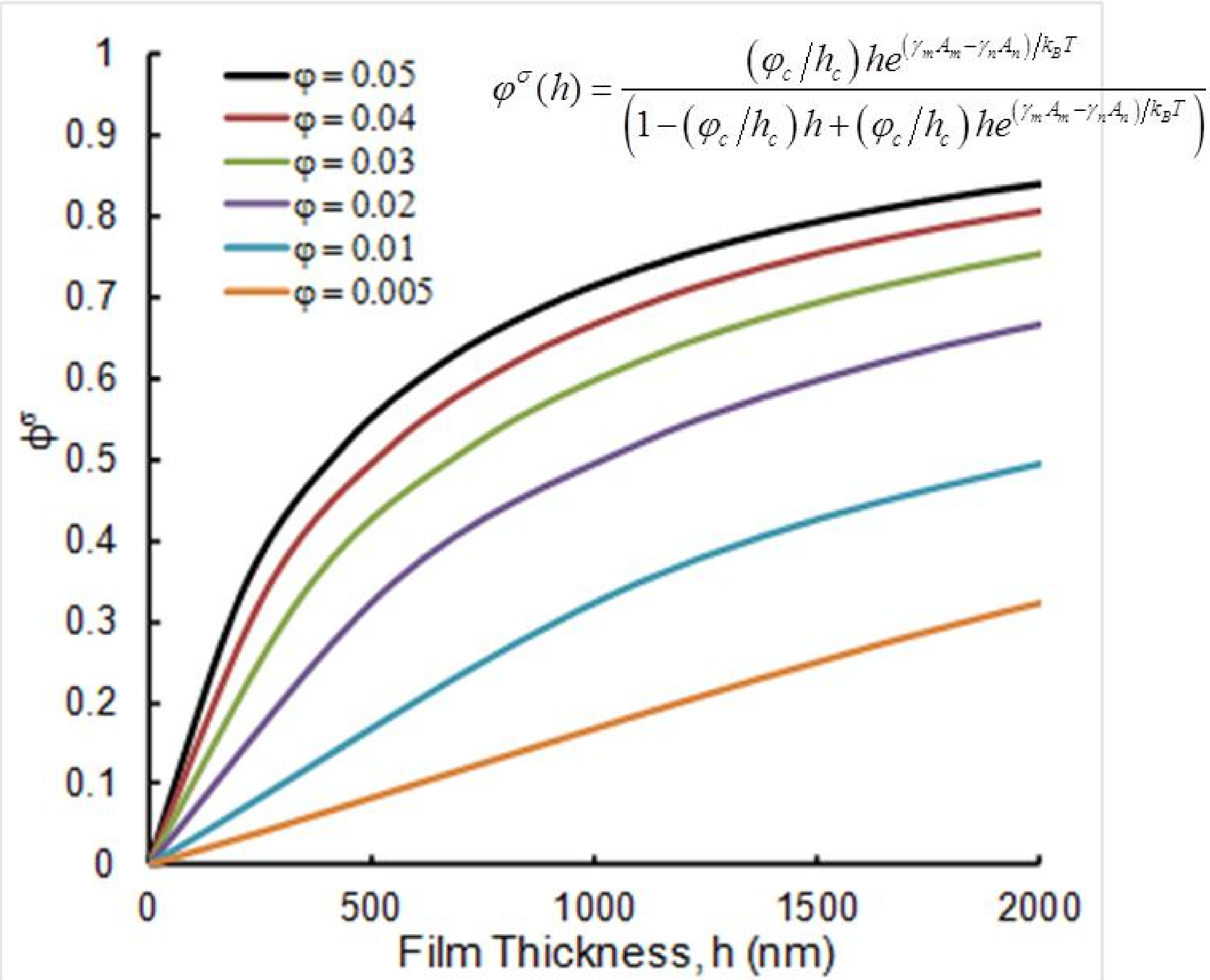
$$\mathcal{F}^{s\sigma} = Nf_n^{s\sigma} + Mf_m^{l\sigma} + k_B T\left[N \ln \varphi_N + M \ln \varphi_M\right]$$



$$\mathcal{F}^{lb} = Nf_n^{lb} + Mf_m^{lb} + k_B T\left[N \ln \varphi_N + M \ln \varphi_M\right]$$

Wax Surface-Freezing in Complex Media

$$\mathcal{A}_m(m^2) = 0.40 \text{ nm } (\mathcal{M}_{asphalt} \sim 150 \text{ Da})$$

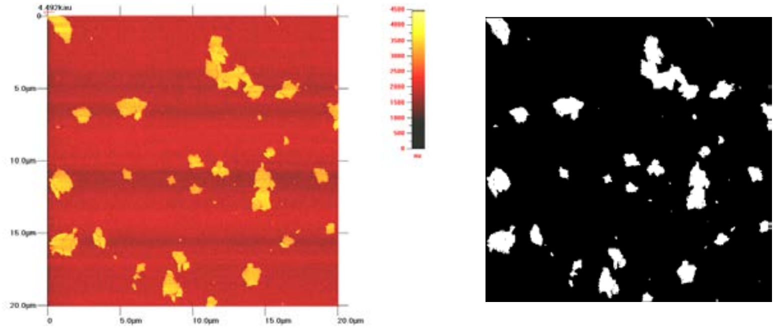


Surface concentration

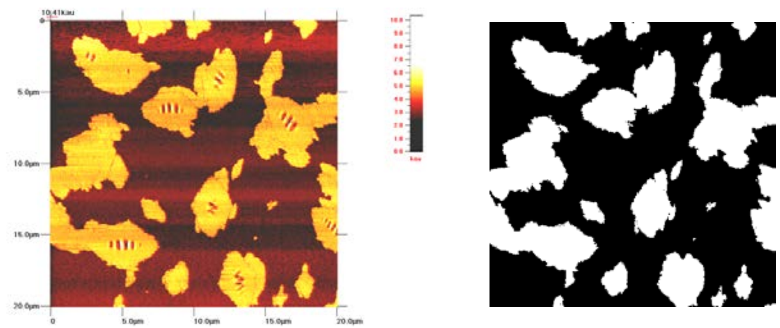
$$\varphi^{\sigma} = \frac{\varphi\Gamma}{1-\varphi+\varphi\Gamma}$$

Bulk concentration

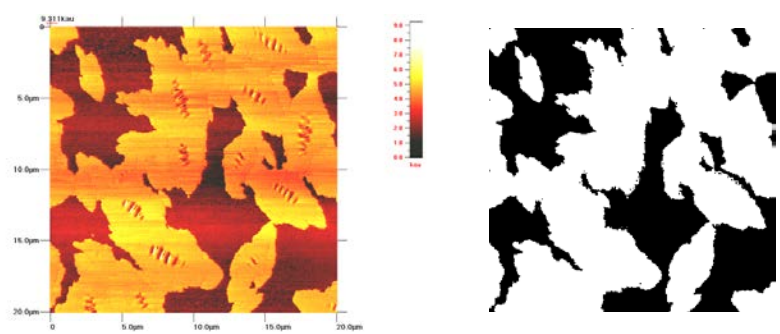
Wax Surface-Freezing in Complex Media



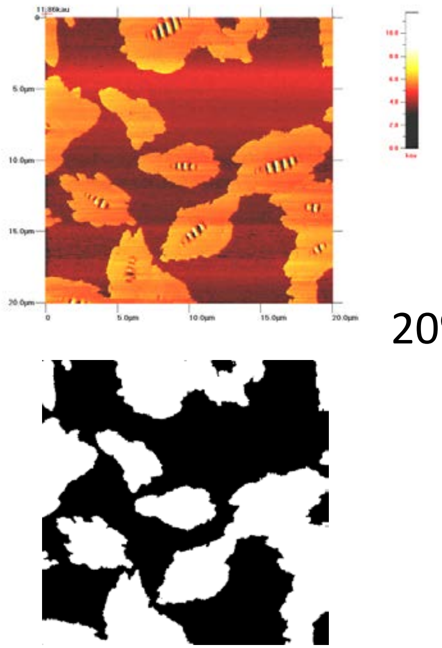
1%



5%



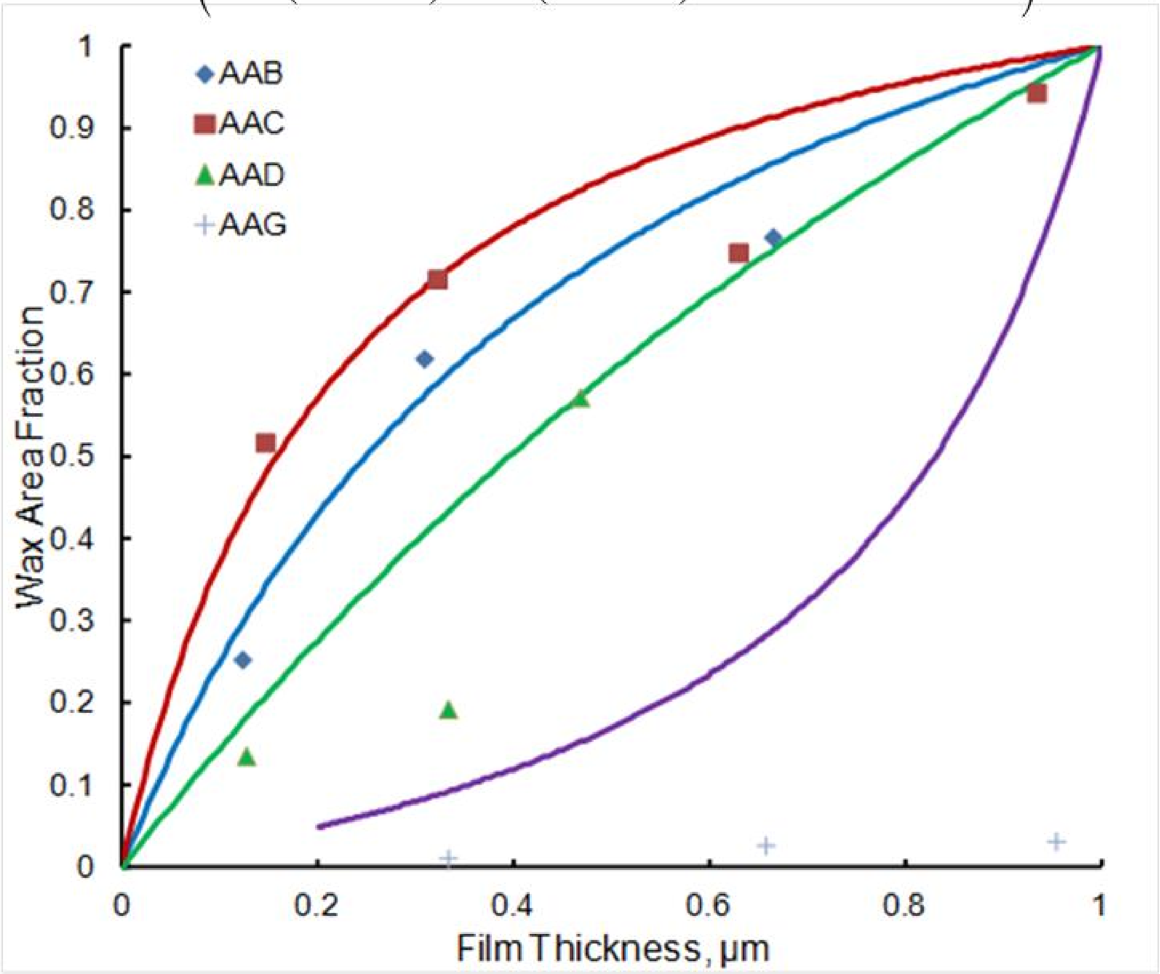
10%



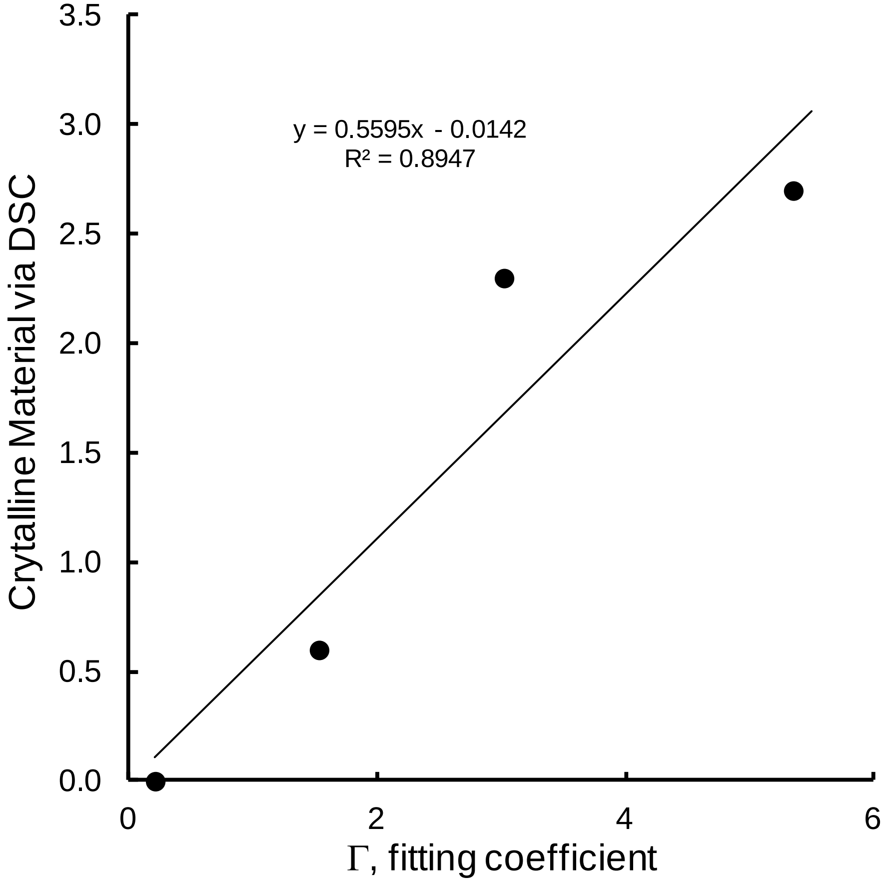
20%

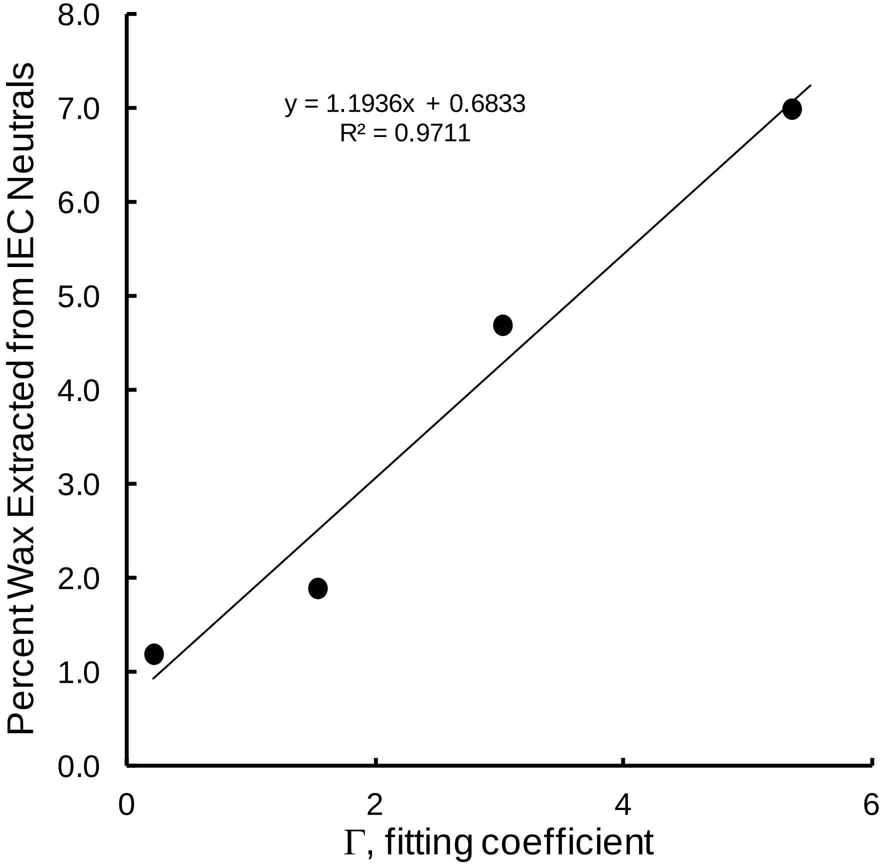
Wax Surface-Freezing in Complex Media

$$\varphi^{\sigma}(h)=\frac{(\varphi_c/h_c)\,he^{(\gamma_m A_m-\gamma_n A_n)/k_BT}}{\left(1-(\varphi_c/h_c)\,h+(\varphi_c/h_c)\,he^{(\gamma_m A_m-\gamma_n A_n)/k_BT}\right)}$$



Wax Surface-Freezing in Complex Media

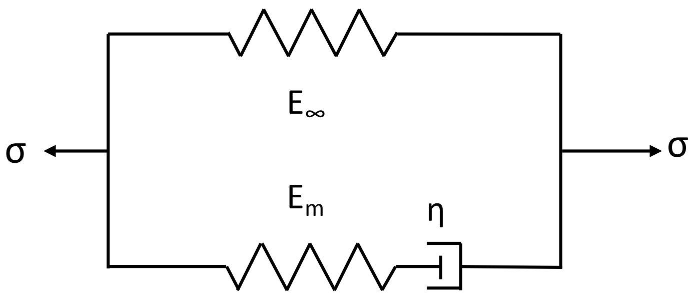




Finite Element Model of Fatigue-Healing Driven by Wax Structuring

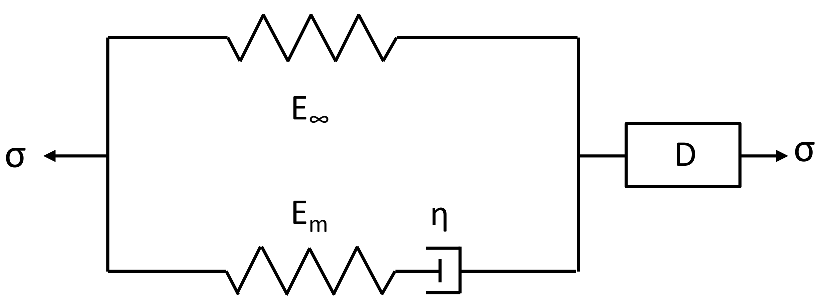
Finite Element Modeling

1 2 3 4 5

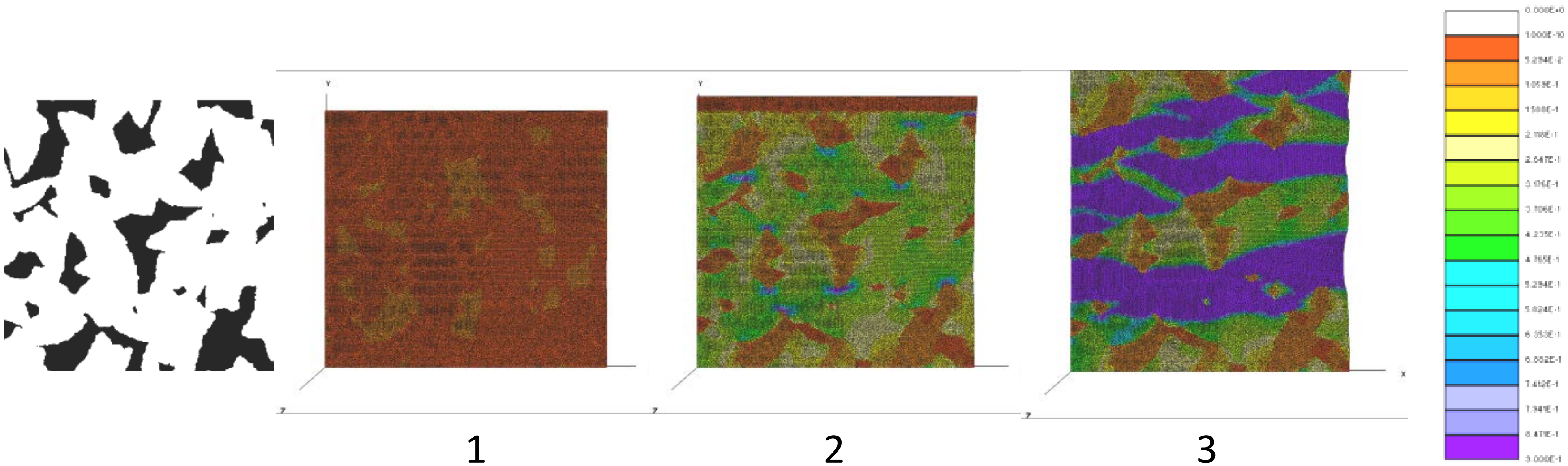


$$T\dot{S}_d = \sum_i X_d J_d$$

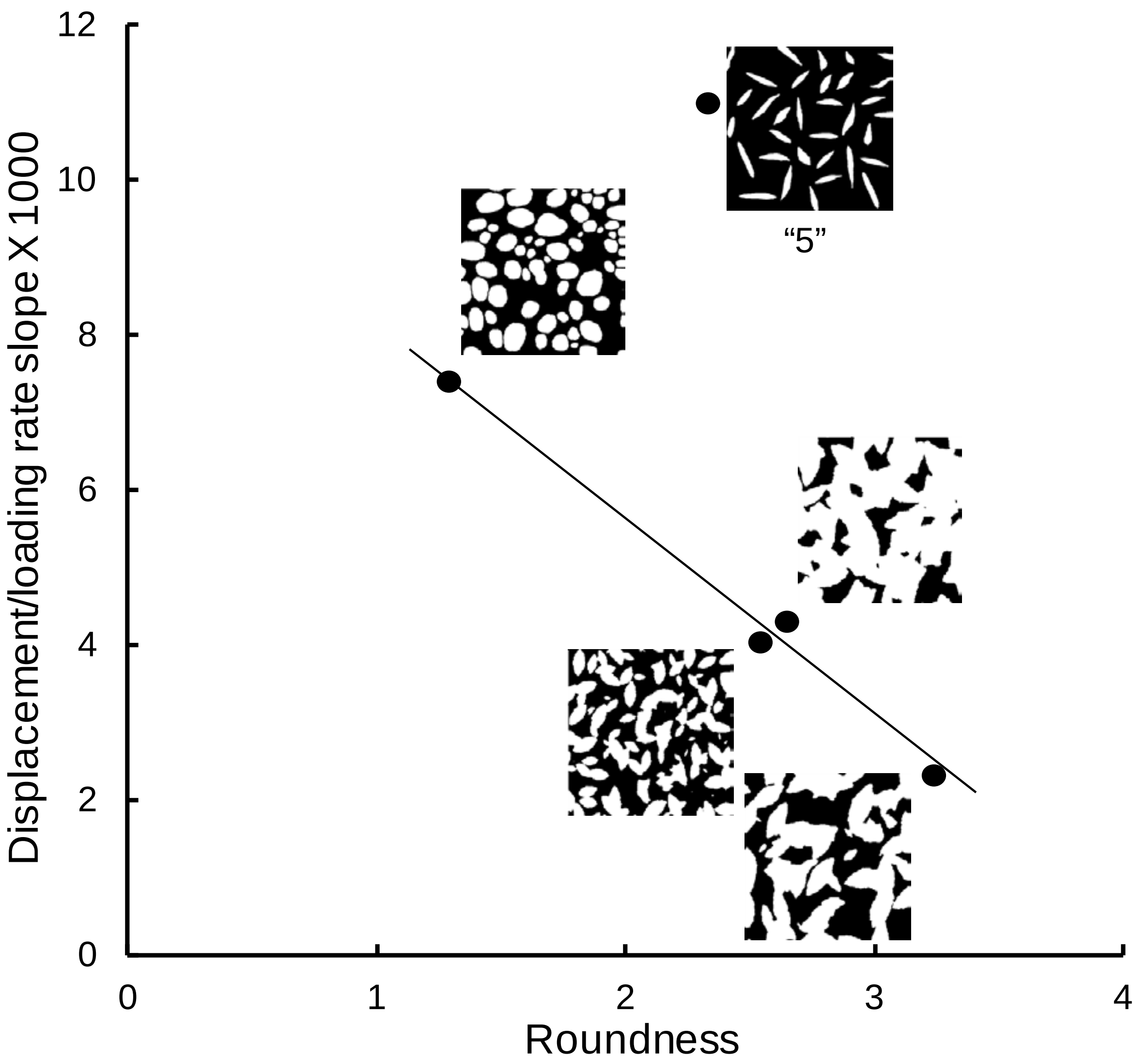
$$= \{\sigma_{ji}\dot{\varepsilon}_{ij} + G_{plastic}\dot{\alpha}\}_d$$



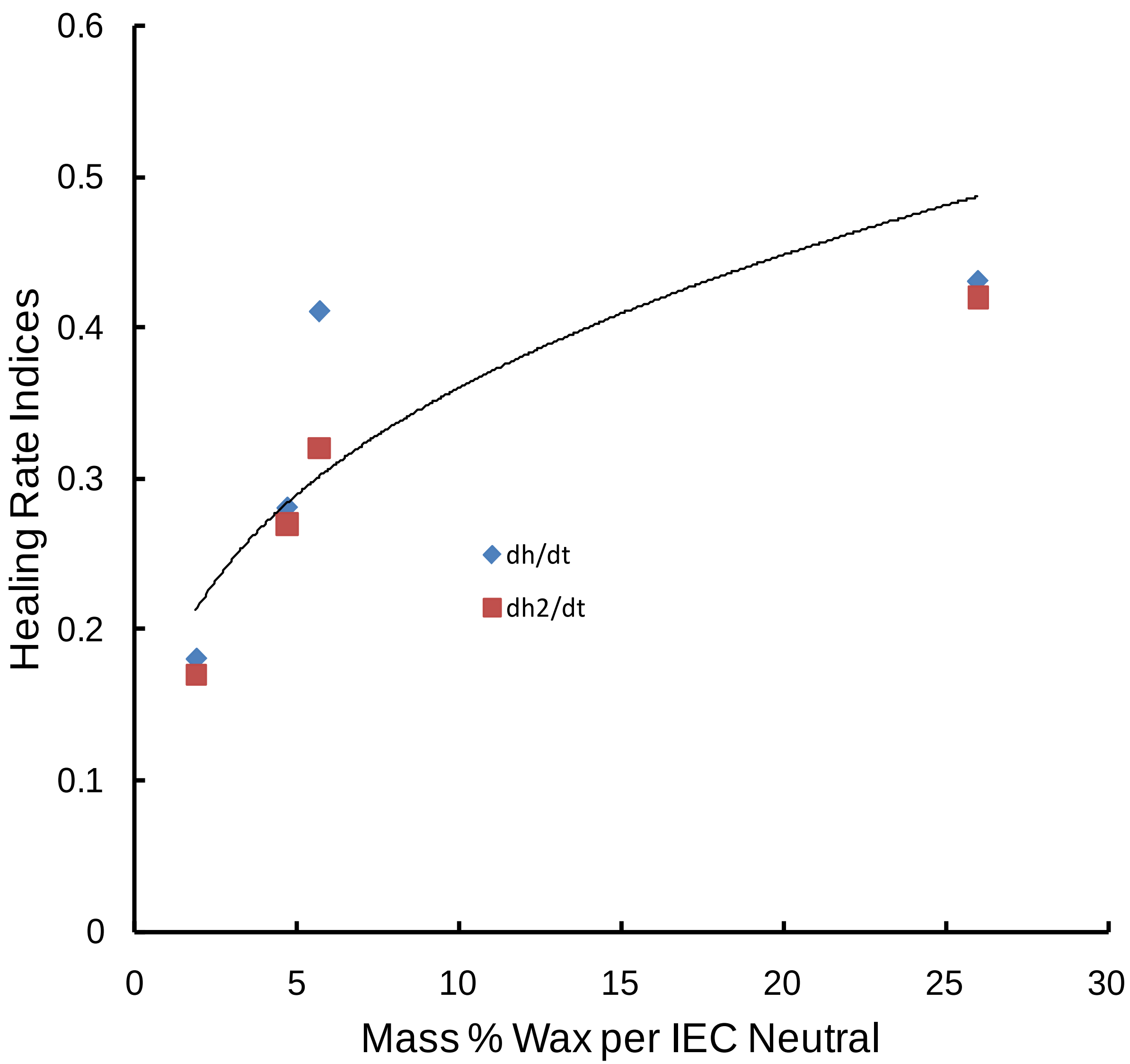
Finite Element Modeling



Finite Element Modeling



Healing and Presence of Wax



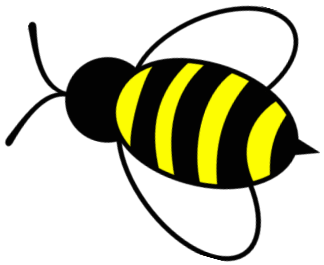
Findings-Conclusions

- The oils phase viscosity is driven by molecular weigh.
- The maltene (i.e., the oils plus resins) may be considered a polar associated solution, BUT, apparent molecular weight may be a big player in viscosity.
- The asphalt (maltene plus asphaltenes) is conveniently modeled as a nano-particle suspension. AGAIN, apparent molecular weight considerations may play a significant role in viscous flow.
- Activation energy models of viscosity work well to explain viscosity-temperature relationships of the nano-particle suspension model considered.
- The Oil's molecular weight correlates with thermal contraction properties of asphalt, thus, thermal fatigue correlates with thermal contraction, ergo, oils molecular weight correlates with , thermal fatigue.
- Asphaltene content strongly contributes to stiffness of RAP mixtures.

Asphalt Research Consortium

Findings-Conclusions

- The "LIQUID" (behavior) of asphalt relates to fatigue-healing.
- Surface crystallization (Surface Freezing) of paraffin wax in complex media involves diffusion controlled crystallization. Bees are observed in both thermally and solvent treated materials.
- Crystals develop at a liquid-vapor interface due to lowering of the liquid-vapor surface free energy state relative to a liquid-solid + solid-vapor state.
- Oils and wax concentration are mutually related in terms of molecular weight, both of which relate to healing.
- Force-flux Coupling makes it difficult to pin-point a single compositional contributor to binder mechanical (rheological) behavior.
- IN SHROT: *a chemomechanics model of bitumen behavior based in non-equilibrium statistical thermodynamics of asphalt microstructure is proposed to predict damage-healing phenomena.*



Thank you
Questions?